Instability of vortices in quantum mechanics and the Helmholtz-Kelvin theorem

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We consider changes of the topological charge of vortices in quantum mechanics, i.e. changes of the velocity field circulation. Conservation of the topological charge of vortices is often related to the Helmholtz-Kelvin theorem known from classical hydrodynamics of non-viscous fluids. We present analytical examples of creation and annihilation of vortices where assumptions of the theorem are broken by quantum evolution of a wave function.

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Introduction. — Vortices can be found both in classical and quantum physics. One can encounter vortices, for instance, in water that spins around or in the air as a ring of smoke [1]. Quantum mechanics can be formulated in a language of hydrodynamics (see e.g. [2,3] and references therein). Such a formulation (very useful also in quantum chemistry [2]) provides a basis for definition of topological defects like vortices [4], whose features are even more striking than those that we find in classical physics. Quantum vortices, however, appear not only in systems described by linear Schrödinger equation. Indeed, they were experimantally observed in superfluid HeII [5] and a Bose-Einstein condensate (BEC) of trapped alkali atoms [6,7] which are typically described, within the mean-field approximation, by the Gross-Pitaevskii equation [8].

In hydrodynamics of ordinary non-viscous fluids, the circulation of the velocity field is conserved in time evolution due to the celebrated Helmholtz-Kelvin theorem (HKT) [9]. This theorem is often employed in quantum mechanics [3,4,10,11]. Nevertheless, uncritical usage of the HKT for quantum systems, may lead to the incorrect conclusion that stability of vortices and vortex rings in a Bose-Einstein condensate is fully guaranteed by the HKT [11]. In the present paper we discuss the basic assumptions of the HKT and show that they can be easily broken by quantum evolution of a wave function, leading to changes of the topological charge. This confirms the recent observation [12] that the topological charge should not be regarded as a fundamental conserved quantity of a quantum system.

Hydrodynamical formulation of quantum mechanics. — To establish connections between quantum mechanics and fluid dynamics we write the wave function in the form $\Psi(\vec{r},t) = \sqrt{\rho(\vec{r},t)}\exp(i\chi(\vec{r},t))$ [2], (where $\rho(\vec{r},t)$ stands for density of a probability fluid) and define the velocity field

$$\vec{v} = \frac{\hbar}{m}\vec{\nabla}\chi(\vec{r},t). \tag{1}$$

Provided $\vec{v}$ and its partial derivatives are well defined, we may rewrite the Schrödinger equation [with a potential $V(\vec{r},t)$] in the form

$$m\frac{\partial\vec{v}}{\partial t} + \vec{\nabla}\left(\frac{1}{2}mv^2 + V - \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}\right) = 0, \tag{2}$$

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot(\vec{v}\rho) = 0. \tag{3}$$

Equation (3) is an ordinary continuity equation, while Eq. (2), in the limit of $\hbar \to 0$, becomes similar to the dynamical equation of a curl-free non-viscous fluid [9].

In quantum mechanics the wave function has to be single valued. To ensure this condition one arrives at the Feynman-Onsanger quantization condition [13] for the circulation of the velocity field Γ_C around any closed contour C

$$\Gamma_C = \oint_C \vec{v}\cdot d\vec{l} = n\frac{2\pi\hbar}{m}, \tag{4}$$

where $n = 0, \pm1, \pm2, \ldots$. Due to the definition (1), we may not expect $n \neq 0$ unless at a certain point on a surface encircled by the contour C, $\vec{\nabla}\times\vec{v}$ becomes singular (behaves as a Dirac delta function, see for example [5]). We refer to n as a topological charge since any continuous deformation of the contour C, which does not incorporate any other points where curl of the velocity field does not vanish, can not change Γ_C.

The Helmholtz-Kelvin theorem. — One may ask whether the circulation Γ_C is conserved in time evolution of the velocity field. For a fixed contour, a possibly moving vortex may leave an area bounded by the contour and consequently Γ_C changes its value. Thus, the relevant situation we should consider corresponds to the case where we let an initially defined contour evolve in time according to the velocity field.

Parameterizing the initial contour by ξ variable, i.e. $C(t_0) = \{\vec{r}(\xi,t_0)\}$, and employing the equation of motion of a contour

$$\frac{d}{dt}\vec{r}(\xi,t) = \vec{v}[\vec{r}(\xi,t)], \tag{5}$$

yields

$$\frac{d}{dt}\Gamma_{C(t)} = \oint_{C(t)} \left(\frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{v} + \frac{1}{2}\vec{\nabla}v^2 \right) \cdot d\vec{l}. \quad (6)$$

If the contour is drawn through points where the velocity field $\vec{v}$ and its partial derivatives are well defined, applying: Eq. (2), equality $(\vec{v}\cdot\vec{\nabla})\vec{v} = \frac{1}{2}\vec{\nabla}v^2 - \vec{v}\times(\vec{\nabla}\times\vec{v})$, and using the fact that, at least on the contour $\vec{\nabla}\times\vec{v} = 0$, we get

$$\frac{d}{dt}\Gamma_{C(t)} = 0. \quad (7)$$

Equation (7) establishes the Helmholtz-Kelvin theorem originally proved for a non-viscous fluid [9].

The HKT is fulfilled provided the contour $C(t)$ that goes initially through points where the velocity field is well defined will evolve in time through such points only. In the following we will see that it is not generally true. Indeed quantum evolution of a wave function, even of a very simple system, may break this assumption leading to a change of the topological charge.

The mean field description of a Bose-Einstein condensate leads to a nonlinear Schrödinger equation — the so-called Gross-Pitaevskii equation [8]. The hydrodynamical formulation of such a problem results in an additional term (proportional to the density ρ) in the bracket of Eq. (2) [8]. However, Eq. (7) still holds (provided, as previously, that a contour $C(t)$ does not go through a singularity).

Analytical examples. — In Ref. [12] the authors show the instability of a vortex placed in an anisotropic two-dimensional harmonic trap. We would like to discuss the source of violation of the HKT in such an instability. We will calculate the velocity field in that system and analyze changes of its circulation from a point of view of the HKT.

Consider an anisotropic two-dimensional harmonic oscillator with the potential

$$V(x,y) = \frac{1}{2}x^2 + \frac{\lambda^2}{2}y^2, \quad (8)$$

(where we use the units of the harmonic oscillator corresponding to the x-direction). The initial wave function is prepared as a superposition of the two lowest excited states

$$\Psi(x,y) \propto (x + i\alpha y)e^{-(x^2+\lambda y^2)/2}, \quad (9)$$

with a real parameter $\alpha > 0$. Choosing any contour C that encircles the origin of the coordinate frame we find out that the circulation $\Gamma_C = 2\pi$ (in harmonic oscillator units). However, the circulation around that point is not conserved in time. Indeed, analysis of time evolution of the velocity field of the system,

$$\vec{v}(x,y,t) = \frac{\alpha \ \cos(Et)}{x^2 + y^2 \ \alpha^2 + 2\alpha xy\sin(Et)}(-y\vec{e}_x + x\vec{e}_y), \quad (10)$$

(where $E = \lambda - 1$ is the energy difference of the two lowest excited states) reveals that for $Et \in [0, \pi/2)$, $\Gamma_C = 2\pi$ while for $Et \in (\pi/2, \pi]$, $\Gamma_C = -2\pi$.

To discuss applicability of the HKT we have to investigate time evolution of the initially defined contour. At any time the velocity (10) is singular at the origin of the coordinates. Thus, if the contour encircles initially the origin, it may not stop doing so – otherwise it crosses the singular point and the integral in Eq. (6) becomes undefined. On the other hand, the evolving contour will go through a singularity anyway as for $Et = \pi/2$, the wave function possesses a nodal line $x + \alpha y = 0$. For $Et = \pi/2 - \varepsilon$ (where $\varepsilon \to 0^+$) the velocity field goes to zero everywhere except on the nodal line where $\vec{v} \to \frac{1}{\varepsilon x}(\vec{e}_x + \alpha\vec{e}_y)$. The HKT can not be, thus, applied in the considered example because quantum evolution of the wave function pushes an evolving contour to singular points and the quantities involved in the theorem become undefined.

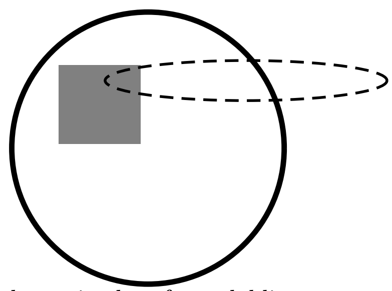

FIG. 1. Schematic plot of a nodal line corresponding to a vortex ring (so
line). In last stage of time evolution the ring shrinks to a point and the c

Another example, we would like to comment on, comes from Ref. [4] where creation and annihilation of a vortex ring for freely moving particle is presented. Even though it is not clearly stated in Ref. [4], the HKT is not fulfilled in that case. The wave function of a vortex ring [4] (in dimensionless units) may be written in the form

$$\Psi(x,y,z,t) \propto [(x-kt)^2 + y^2 + z^2 - 1 + i3(z+t)]e^{ikx - ik^2t/2}, \quad (11)$$

where the wave vector $\vec{k} = (k, 0, 0)$ is related to a motion of the "center of mass" of the vortex ring with a constant velocity $\vec{k}$. The vortex ring corresponds to the nodal line of the wave function and is located at the intersection of the plane $z + t = 0$ and sphere $(x - kt)^2 + y^2 + z^2 = 1$. At time $t = -1$, the vortex is born at a point $(-k, 0, 1)$ and, at time $t = 1$, it disappears at a point $(k, 0, -1)$. The radius of the vortex changes in time as $\sqrt{1 - t^2}$.

Suppose at any time $t \in (-1, 1)$, we define a contour C so that it encircles the vortex (see Fig. 1) and the circulation of the velocity field corresponds to $n = 1$. The evolving contour can not cross the vortex ring without facing a singularity in the velocity field. However, the ring at some moment starts shrinking and at $t = 1$ it reduces to a point. Consequently, at $t = 1$, the contour must go through a singularity of the velocity field and the integral (6) and also the HKT become meaningless.

Now we would like to consider example corresponding to a driven two level system. Consider, for simplicity, a two-dimensional H atom initially in the first excited state (with angular momentum $L = 1$) that is driven resonantly by a circularly polarized electromagnetic field. The field frequency ω is tuned to the transition between the first and second excited energy states (i.e. $\omega = E_2 - E_1$, where E_1 and E_2 stand for the energy of the first and second excited states, respectively). Therefore, we may restrict the description of the system to a two-dimensional Hilbert space: $\psi_1(r,\varphi) \propto r\exp(-2r/3)\exp(i\varphi)$ and $\psi_2(r,\varphi) \propto r^2\exp(-2r/5)\exp(i2\varphi)$, with the Schrödinger equation (in the atomic units)

$$i\frac{d}{dt}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} E_1 & De^{i\omega t} \\ De^{-i\omega t} & E_2 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix}, \qquad (12)$$

where D is a dipole matrix element [14]. The solution of Eq. (12) reveals Rabi oscillations [14] of the populations [$C_1(t)$ and $C_2(t)$] of the unperturbed atomic states that correspond to a change of the topological charge of vortices in the system. For $t = 0$ there is a vortex with $n = 1$ at the center of the coordinates as expected for the state with angular momentum $L = 1$ [$C_1(0) = 1$]. When Dt increases another vortex with $n = 1$ moves in from *infinity*, collides with the first one (situated at the center of the coordinates) for $Dt = \pi/2$ and then moves out to *infinity* again and so on. In the configuration space, in the frame rotating with the frequency ω, the radial position of the moving vortex is given by solution of the following equation

$$r\exp(4r/15) = \frac{125\sqrt{5}}{18}\left|\frac{\cos(Dt)}{\sin(Dt)}\right|, \qquad (13)$$

while the angular position is: $\varphi = -\pi/2$ for $Dt \in (0, \pi/2)$ and $\varphi = \pi/2$ for $Dt \in (\pi/2, \pi)$ — in the laboratory frame it corresponds to motion along spiral lines. During the collision, i.e. for $Dt = \pi/2$, a single vortex with $n = 2$ is formed. In the considered example, the HKT may not apply if we define a contour so that it encircles only one vortex with $n = 1$. Indeed, such a contour either moves out to *infinity* or encounters a singularity in the velocity field during a "collision" with the other vortex. It is interesting to note that the $n = 2$ topological charge is possible in an ideal case only when there is no contribution of the $\psi_1(r,\varphi)$ state to the wave function.

Summary and conclusions. — We have analyzed the applicability of the Helmholtz-Kelvin theorem to the hydrodynamical formulation of the quantum mechanics. The velocity field of the probability fluid is defined as a gradient of a phase of a quantum wave function. This implies that nonzero circulation, along a given contour, may come out in the system if the field reveals a singularity at certain points on a surface encircled by the contour. Adopting the HKT to the quantum liquid may suggest that such a topological charge of the system can not change.

However, the HKT may be employed if a given contour evolves through points where the velocity field is well defined. This is not generally true in a quantum system — especially a singularity is necessary for a nonzero circulation. We have presented simple analytical examples where the quantum evolution of a wave function pushes a contour to a singular point. Such a process is accompanied by a change of the topological charge that illustrates instability of vortices.

The main result of this work states that stability of vortices can not be guaranteed by the Helmholtz-Kelvin theorem — that theorem may not work even for simple systems. Therefore the theorem becomes useless in quantum mechanics.

Mean field description of a Bose-Einstein condensate of interacting atoms leads to a nonlinear Schrödinger equation, i.e. the Gross-Pitaevskii equation. We show that conclusions concerning the HKT that are drawn from the analysis of linear quantum mechanics remains valid also for the nonlinear problem. However, introducing the interaction between atoms can change dynamics of vortices. For example, in a linear problem, circulation of the velocity field corresponding to the vortex placed at the center of an anisotropic harmonic potential reveals periodic changes of sign [12]. However, appearance of nonlinearity in the corresponding Schrödinger equation makes the vortex at the center stable [12]. It suggests that the nonlinear dynamics (not HKT) is responsible for the stability of the vortex in that example.

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[1] R. P. Feynman, R. B. Leighton, M. Sands, The Feynman Lectures on Physics, Volume II, (Addison-Wesley Publishing Company, Massachusetts, 1963).
[2] S. K. Ghosh, B. M. Deb, Phys. Rep. **92** 1 (1982).
[3] I. Białynicki-Birula, M. Cieplak, and J. Kaminski, Theory of Quanta (Oxford University Press, Oxford, 1992).
[4] I. Białynicki-Birula, Z. Białynicka-Birula, and C. Śliwa, Phys. Rev. A **61** 032110 (2000).
[5] E. L. Andronikashvili and Yu. G. Mamaladze, Rev. Mod. Phys. **38** 567 (1966).
[6] M. R. Matthews, B. P. Anderson, P. C. Haljan, D. S. Hall, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. **83**, 2498 (1999).
[7] K. W. Madison, F. Chevy, W. Wohlleben, and J. Dalibard, Phys. Rev. Lett. **84**, 806 (2000).
[8] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari Rev. Mod. Phys. **71** 463 (1999).

[9] L. D. Landau, E. M. Lifszyc, Fluid Mechanics (Butterworth-Heinemann, 1995).
[10] E. L. Bolda and D. F. Walls, Phys. Rev. Lett. **81** 5477 (1998).
[11] B.P. Anderson, P. C. Haljan, C. A. Regal, D. L. Feder, L. A. Collins, C. W. Clark, and E. Cornell, Phys. Rev. Lett. **86** 2926 (2001).
[12] J. J. García-Ripoll, G. Molina-Terriza, V. M. Perez-García, and L. Torner, Phys. Rev. Lett. **87** 140403 (2001).
[13] R. P. Feynman, Statistical Mechanics, (W. A. Benjamin, Massachusetts, 1972).
[14] C. Cohen-Tannoudji, J Dupont-Roc, G. Grynberg, Atom-Photon Interactions: Basic Processes and Applications (John Wiley & Sons, 1992).